TRANSFORMATION OF TWO AND THREE-DIMENSIONAL

REGIONS BY ELLIPTIC SYSTEMS

Semiannual Status Report
for the period
April 1, 1991 through September 30, 1991

submitted under

by

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October 31, 1991

1 Progress Report

The major accomplishment during this contract period has been the incorporation of the multiblock derivative interface algorithm into the flux-split Euler code developed here at MSU. The code can now be used to compute flow on any multiblock configuration provided the block boundary surfaces coincide. There is no need for any type of grid line or slope continuity at the block boundaries. We do not permit the overlapping of blocks so that all interpolation can be done on surfaces, which is a two- dimensional interpolation problem. Since our Euler code is a cell-centered scheme, there arose some unexpected problems as to how the phantom points should be updated. This is mainly a problem with the second-order scheme where there are two surrounding layers of phantom points that must be updated after each time step. After trying several alternatives, it was decided that linear extrapolation from the values on the block boundary worked best. These problems did not arise with the MacCormack method that was used in our earlier developmental work. One of our concerns in the earlier work with this interface procedure was whether the updating at the boundary could be done efficiently. The update procedure is an implicit algorithm and the boundary values are computed at each time step using an ADI scheme. In a three-dimensional test case, it was observed that the number of ADI iterations has practically no effect on the numerical solution. Therefore, we are using only one ADI iteration per time step. Thus, in terms of operation count, the update procedure is competitive with any explicit procedure. It should be noted that these conclusions are preliminary since we only recently began computations on three- dimensional multiblock grids.

The following example is included to illustrate the type of results that have been seen. The geometry is a simple three- dimensional axisymmetric body with a spherical grid system. A supersonic flow is computed with a zero angle of attack. Discontinuities in grid lines occurs when the grid is refined near the leading and trailing edges. The contours appearing in the following figure were plotted from a solution computed using the derivative interface procedure. As a check on the procedure, a solution was also computed by extending the grid lines into the neighboring block and interpolating solution values. There was no noticeable difference in the two solutions.

The presentation "Derivative Interface Conditions for Multiblock Grids" made at the Third International Conference on Numerical Grid Generation in
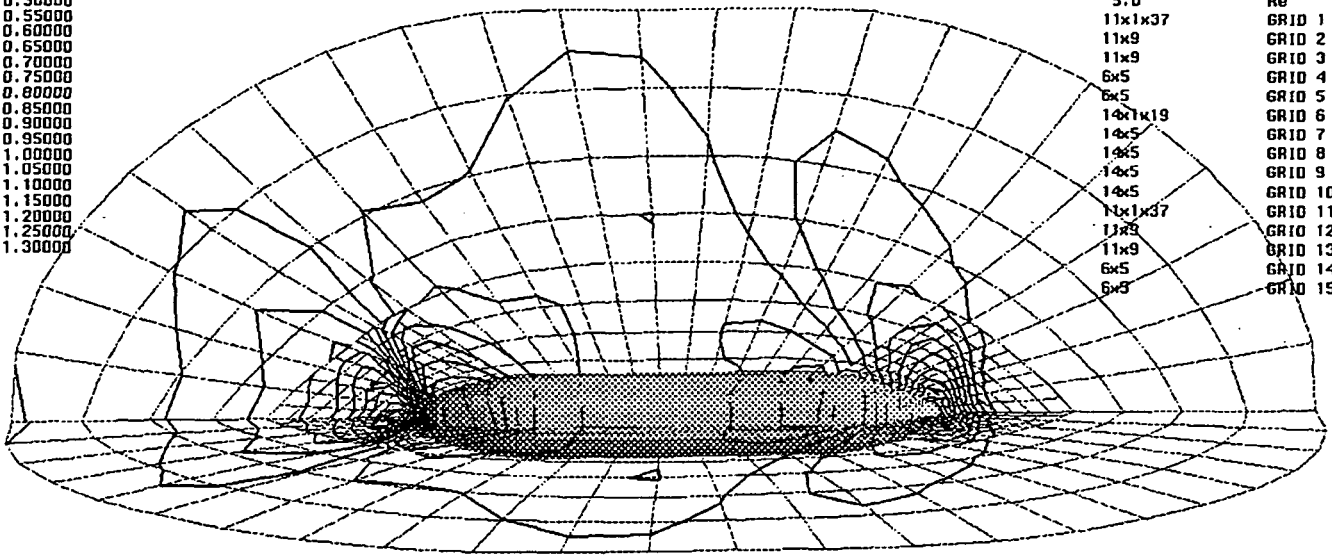
Figure 1: Interface procedured applied to a three-dimensional grid with grid line discontinuity

Barcelona included our results as of June 1991. The paper which appeared in the Proceedings was submitted earlier in the spring and was attached to our last semiannual report. We have included with this report the paper entitled "Linear Variational Methods and Adaptive Grids". The paper was recently accepted for publication in *Computers and Mathematics with Applications*. The manuscript was submitted over a year ago and contains work that was done about two years ago. However, since there is now a renewed interest in variational methods, the work is still timely.

Linear Variational Methods and Adaptive Grids

C. Wayne Mastin *

1 Introduction

The progression of larger and larger supercomputers has not eliminated the need for adaptive grids in computational fluid dynamics. Instead, it has brought demands for more detailed resolution in the flow field and the solution of more complicated fluid flow problems. Regardless of the chosen algorithm, the resolution of shock waves and boundary layers demands extremely close spacing of grid points. Shock waves can be especially difficult to deal with because they appear in the interior of the computational region and may be a transient phenomena.

The adaptive grids considered in this report will be structured grids and will be constructed by moving existing grid points into regions where solution variables have large derivatives. In recent years the term adaptive grid has expanded to encompass such topics as local grid refinements and fine grid overlays. These techniques can be used without having to deal with problems of grid distortion, but they do require an additional level of data structure and cannot be easily incorporated into an existing grid generation / flow solver package.

The redistribution of grid points in the construction of adaptive grids can be done using either direct algebraic methods or iterative methods that are derived from variational problems or elliptic boundary value problems. Algebraic methods are the simplest and generally involve a spline fit of the points based on some equidistribution principle. As with all algebraic methods, there is no way of insuring against grid folding (negative Jacobians), especially if the redistribution is done in more than one coordinate direction. Iterative methods for constructing adaptive grids have now been used

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routinely for several years. The initial work on the variational based methods was done by Brackbill and Saltzman [3]. The foundations for the most popular elliptic method were laid by Anderson and Steinbrenner [1] using the system of elliptic partial differential equations developed by Thompson *et al* [9]. Presently the equations of Anderson and Steinbrenner are most widely used for three-dimensional problems since the Euler equations for the variational method are very lengthy.

Comprehensive review articles on adaptive grids have been written by Eiseman [5] and Thompson [8]. The elliptic grid generation equations of Thompson are accepted as the best system for constructing arbitrary curvilinear grids. There is only one problem that may arise in implementing the method. The elliptic equations which must be solved numerically are nonlinear and iterative methods for solving the equations do not always converge. This is particularly true in the case of adaptive grid construction where there are large variations in grid spacing. The nonlinearity also implies that numerical algorithms will only be locally convergent and, therefore, convergence will only occur if the iterative sequence starts with a reasonable estimate of the final grid. While none of these problems are insurmountable, it has lead to an interest in grid generation methods based on the solution of linear systems of algebraic equations. Linear algebraic equations may be derived from the discretization of linear systems of partial differential equations or from the direct discretization of certain variational problems. Most recently work in this area has been reported by Castillo *et al* [4]. A somewhat similar approach was followed by Kennon and Dulikravich [6]. The latter method was based on a discrete optimization problem while the former considered a continuous variational problem. Depending on the discretization used in the variational problem, the methods may or may not generate the same system of linear algebraic equations. A comparison of grids generated by linear and nonlinear methods can be found in the reports of Castillo *et al* and Mastin *et al* [7].

The objective of this report is to derive linear systems for grid generation which naturally tend to generate nonfolding grids. The key to the method is to attempt to preserve the aspect ratios of the grid cells when transforming between the physical and computational regions. Surprisingly, this fact was noted many years ago by Barfield [2]. Only two-dimensional grids were considered, in which case the appropriate generating equations can be derived from properties of conformal mappings. The same equations will be derived here in a slightly different way which leads to grid generating equations in three dimensions and also equations for construct-

ing two and three-dimensional adaptive grids. Examples have demonstrated that nonfolding grids can be constructed for many nonconvex regions where methods that use smoothing formulas derived from Laplace's equation fail. The adaptive grids constructed using linear methods are similar to those constructed by nonlinear methods and are more orthogonal in some cases. However, the methods which are presented here should not be considered as a replacement for existing elliptic and variational schemes. There were cases where they failed to generate a satisfactory grid while the existing nonlinear schemes were successful. On the other hand, they are still attractive because all the traditional iterative schemes to solve the linear systems of algebraic equations will always converge regardless of the initial grid coordinates.

2   Two-Dimensional Grid Generation

The variational approach will be used to generate the difference equations. This leads directly to the generalization to three dimensions and the equations for adaptive grids. Since one of the problems in the construction of adaptive grids is skewness, the development will begin with the variational principle of conformal mappings.

The adaptive grid will be constructed from the mappings in Figure 1. An arbitrary bounded simply-connected region R in the xy-plane can be conformally mapped onto a rectangular region with four given points of R mapping to the vertices of the rectangle. If one of the mapping functions is scaled, the resulting transformation maps R onto a square S. The aspect ratio of the rectangular region is a conformal invariant of R called its module and denoted by M. The transformation from the square onto R minimizes the following integral

$$\iint_S M(x_\mu^2 + y_\mu^2) + \frac{1}{M}(x_\nu^2 + y_\nu^2)\,d\mu d\nu. \tag{1}$$

The conformal mapping also satisfies boundary orthogonality constraints which will not be considered in this development. One-dimensional stretching transformations can be composed with conformal mappings without destroying the one-to-one and orthogonality properties of the mapping. Thus, one-dimensional transformations defined by the equations

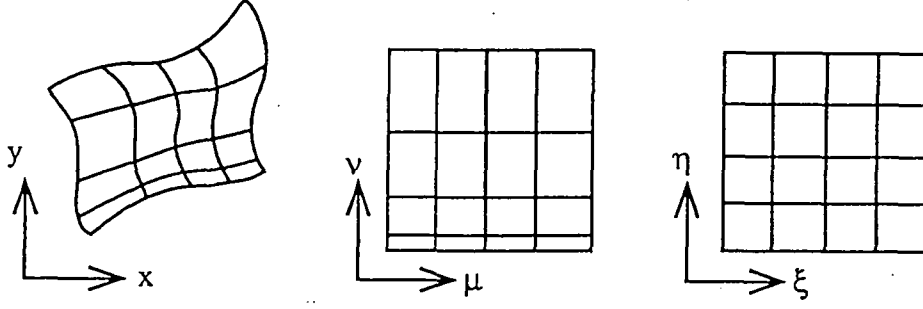$$\mu = a(\xi),\ 0 \leq \xi \leq 1$$
$$\nu = b(\eta),\ 0 \leq \eta \leq 1$$

Figure 1: Composite Mappings for a Two-Dimensional Grid

will be included in the mapping from the square onto the region R. The resulting transformation minimizes the integral

$$\iint_S M \frac{b'(\eta)}{a'(\xi)}(x_\xi^2 + y_\xi^2) + \frac{1}{M}\frac{a'(\xi)}{b'(\eta)}(x_\eta^2 + y_\eta^2)\, d\xi d\eta. \qquad (2)$$

One of the objectives of an adaptive grid is to equidistribute some quantity over the total region. The transformations a and b can be chosen from an equidistribution property. Suppose that $f(\xi)$ is a positive function defined for $0 \le \xi \le 1$. A one-dimensional mapping will equidistribute the function f on the unit interval if

$$f(\xi)\, d\mu = c\, d\xi,$$

where c is a constant to be determined. The equation can also be written as

$$a'(\xi) = \frac{c}{f(\xi)}. \qquad (3)$$

Integrating from $\xi = 0$ to $\xi = 1$ gives

$$1 = \int_0^1 \frac{c}{f(\tau)} d\tau$$

4

or

$$c = \left(\int_0^1 \frac{1}{f(\tau)} d\tau \right)^{-1}.$$

Therefore, an equidistribution of $f(\xi)$ in the $\mu\nu$-plane can be accomplished from the one-dimensional stretching transformation given by the above differential equation or explicitly as

$$a(\xi) = c \int_0^\xi \frac{1}{f(\tau)} d\tau.$$

Since the mapping from the $\mu\nu$-plane to the xy-plane is generated from properties of conformal mappings, the resulting grid will also locally exhibit an approximate equidistribution property. An equidistribution in the other coordinate direction would be done by choosing the function $b(\eta)$ in a similar fashion. If orthogonality is essential, then the adaptivity functions are restricted to one-dimension. However, since the orthogonality condition is not really our aim, two-dimensional equidistribution functions will be allowed so that the integral in (2) can be generalized. Two functions $f(\xi, \eta)$ and $g(\xi, \eta)$ will be considered with f controlling adaptation in the ξ-direction and g controlling adaptation in the η-direction. It will be assumed that these functions have been normalized along grid lines so that the constant in (3) is at least approximately $c = 1$. The adaptive grid is constructed by minimizing the integral

$$\iint_S M \frac{f(\xi, \eta)}{g(\xi, \eta)} (x_\xi^2 + y_\xi^2) + \frac{1}{M} \frac{g(\xi, \eta)}{f(\xi, \eta)} (x_\eta^2 + y_\eta^2) \, d\xi d\eta. \qquad (4)$$

Two things are still needed to make this an easily solvable problem. The boundary correspondence must be given. Equidistribution of a weight function along a curve is a simple algebraic procedure and it will be assumed that this has been done before the interior grid points are to be calculated. No attempt will be made to duplicate the boundary correspondence of the conformal mapping since that would lead to a nonlinear problem. The quantity M must also be calculated. Computational experience has shown that only a crude approximation is necessary. If this grid generation scheme is to be an iterative scheme, the initial grid may be an algebraic grid on R. In that case one could compute an average aspect ratio of all cells of the algebraic grid. Using the mapping notation, we would compute M as

$$M = \iint_S \left[\frac{x_\eta^2 + y_\eta^2}{x_\xi^2 + y_\xi^2} \right]^{\frac{1}{2}} d\xi d\eta.$$

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where

$$
\begin{aligned}
x &= x(\xi, \eta) \\
y &= y(\xi, \eta)
\end{aligned}
$$

is any mapping of the square region onto the region R. A simpler procedure which avoids the need for an initial algebraic grid is to define M as the ratio of the average lengths of opposite sides of R.

A discretization of the integral (4) leads to a least-squares problem which in turn yields linear equations for the coordinates x and y. Since both equations are the same, we let $\vec{r} = (x,y)$, i and j denote the grid point indices, and write the system as

$$
\begin{aligned}
P_{i+\frac{1}{2},j}(\vec{r}_{i+1,j} - \vec{r}_{i,j}) + P_{i-\frac{1}{2},j}(\vec{r}_{i-1,j} - \vec{r}_{i,j}) \\
+ Q_{i,j+\frac{1}{2}}(\vec{r}_{i,j+1} - \vec{r}_{i,j}) + Q_{i,j-\frac{1}{2}}(\vec{r}_{i,j-1} - \vec{r}_{i,j}) &= 0
\end{aligned}
$$

where

$$
\begin{aligned}
P_{i\pm\frac{1}{2},j} &= \frac{\Delta\eta \, f_{i\pm\frac{1}{2},j}}{\Delta\xi \, g_{i\pm\frac{1}{2},j}} M \\
Q_{i,j\pm\frac{1}{2}} &= \frac{\Delta\xi \, g_{i,j\pm\frac{1}{2}}}{\Delta\eta \, f_{i,j\pm\frac{1}{2}}} \frac{1}{M}.
\end{aligned}
$$

Since P and Q are positive, this linear system of equations for the grid points $(x_{i,j}, y_{i,j})$ is diagonally dominant and can be solved using any direct of iterative method.

It should be noted that this grid adaptation method causes grid clustering by controlling the cell aspect ratio. The same control function cannot be used to cluster simultaneously in the ξ and η directions because if $f = g$, the integral (4) reduces to integral (1). Of course, grid adaptation could be achieved by introducing a weight function in (1), that is, replace $d\mu \, d\nu$ by $w(\mu, \nu) \, d\mu \, d\nu$, but then the method would loose much of the orthogonality inherent in its development.

3   Three-Dimensional Grid Generation

The basic concept in the two-dimensional development is preservation of cell aspect ratios in conformal mappings. Although conformal mappings do not extend to three dimensions, this basic concept can be formulated. The
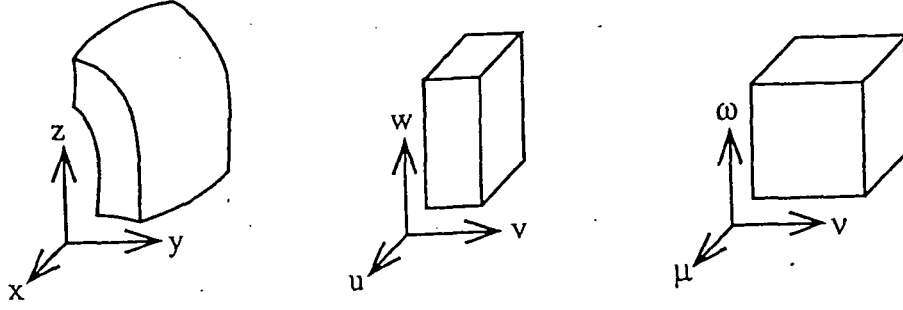
Figure 2: Composite Mappings for a Three-Dimensional Grid

initial assumption is that given a three-dimensional region R, a one-to-one mapping of a rectangular region Q onto R can be found which minimizes the integral

$$\iiint_Q \|\vec{r}_u\|^2 + \|\vec{r}_v\|^2 + \|\vec{r}_w\|^2 \, du \, dv \, dw$$

provided the length, L, width, W, and height, H, of Q are properly defined and suitable boundary conditions are imposed. Although this may seem a plausible statement, no results of this type have been found in the literature and it is doubtful that it is true for all regions. Thus the three-dimensional generalization begins on a less firm footing and the value of the final grid generation algorithm must be judged by its ability to generate nonfolding grids of practical interest.

A sequence of mappings will be examined as illustrated in Figure 2. The first step will be the mapping of the rectangular region Q onto a unit cube, C. This can be done by scaling so that

$$u = L\mu, \quad v = W\nu, \quad w = H\omega.$$

The integral (5) becomes

$$\iiint_C \frac{WH}{L}\|\vec{r}_\mu\|^2 + \frac{LH}{W}\|\vec{r}_\nu\|^2 + \frac{LW}{H}\|\vec{r}_\omega\|^2 \, d\mu \, d\nu \, d\omega \tag{5}$$

In view of our basic assumption it is now evident that the mapping of the unit cube onto an arbitrary region should depend on the dimensions of the region. Here we have three parameters to approximate instead of one as in integral (1). Proceeding as in two dimensions, if an initial grid is given on R from say an algebraic mapping of the cube, then the following ratios can be computed.

$$M_1 = \frac{WH}{L} = \iiint_C \frac{\|\vec{r}_\nu\| \|\vec{r}_\omega\|}{\|\vec{r}_\mu\|} \, d\mu \, d\nu \, d\omega$$

$$M_2 = \frac{LH}{W} = \iiint_C \frac{\|\vec{r}_\mu\| \|\vec{r}_\omega\|}{\|\vec{r}_\nu\|} \, d\mu \, d\nu \, d\omega$$

$$M_3 = \frac{LW}{H} = \iiint_C \frac{\|\vec{r}_\mu\| \|\vec{r}_\nu\|}{\|\vec{r}_\omega\|} \, d\mu \, d\nu \, d\omega$$

Once again the geometric ratios of the region R are approximated by computing the average ratios of all the grid cells in R. Grid adaptivity can also be included by first considering one-dimensional stretching and then generalizing the control functions so that the degree of stretching is allowed to vary between grid lines. If the stretching transformations map the unit cube in $\xi\eta\zeta$-space to the unit cube in $\mu\nu\omega$ -space and the functions to be approximately equidistributed along the ξ, η, and ζ grid lines are f, g, and h, then the integral (6) to be minimized becomes

$$\iiint_C M_1 \frac{f}{gh} \|\vec{r}_\xi\|^2 + M_2 \frac{g}{fh} \|\vec{r}_\eta\|^2 + M_3 \frac{h}{fg} \|\vec{r}_\zeta\|^2 \, d\xi \, d\eta \, d\zeta.$$

Three-dimensional adaptivity can also be achieved by weighting the differential as described in the previous section. A direct discretization of the variational problem leads to the following diagonally dominant linear system.

$$P_{i+\frac{1}{2},j,k}(\vec{r}_{i+1,j,k} - \vec{r}_{i,j,k}) + P_{i-\frac{1}{2},j,k}(\vec{r}_{i-1,j,k} - \vec{r}_{i,j,k})$$
$$+Q_{i,j+\frac{1}{2},k}(\vec{r}_{i,j+1,k} - \vec{r}_{i,j,k}) + Q_{i,j-\frac{1}{2},k}(\vec{r}_{i,j-1,k} - \vec{r}_{i,j,k})$$
$$+R_{i,j,k+\frac{1}{2}}(\vec{r}_{i,j,k+1} - \vec{r}_{i,j,k}) + R_{i,j,k-\frac{1}{2}}(\vec{r}_{i,j,k-1} - \vec{r}_{i,j,k}) \quad = \quad 0$$

where

$$P = \frac{\Delta\eta \, \Delta\zeta \, f}{\Delta\xi \, g \, h} M_1$$

$$Q = \frac{\Delta\xi \, \Delta\zeta \, g}{\Delta\eta \, f \, h} M_2$$

$$R = \frac{\Delta\xi \, \Delta\eta \, h}{\Delta\zeta \, f \, g} M_3$$

4 Conclusions

The objective of this report has been to present a reliable linear system for grid generation in two and three dimensions. The method is robust in the sense that convergence is guaranteed but is not as reliable as other non-linear elliptic methods in generating nonfolding grids. The construction of nonfolding grids depends on having reasonable approximations of cell aspect ratios and an appropriate distribution of grid points on the boundary of the region. Some guidelines have been included on approximating the aspect ratios, but we can offer little help on setting up the boundary grid other than to say that in two dimensions the boundary correspondence should be close to that generated by a conformal mapping.

It has been assumed that the functions which control the grid distribution depend only on the computational variables, ξ, η, and ζ, and not on the physical variables, x, y, and z. Whether this is actually the case depends on how the grid is constructed. In a dynamic adaptive procedure where the grid is constructed in the process of solving a fluid flow problem, the grid is usually updated at fixed iteration counts using the current value of the control function. Since the control function is not being updated during the iteration of the grid equations, the grid construction is a linear procedure. However, in the case of a static adaptive procedure where a trial solution is computed and used to construct an adaptive grid, the control functions may be recomputed at every step of the adaptive grid iteration based on the current location of the grid points. This latter case gives rise to a nonlinear system and convergence cannot be guaranteed regardless of the elliptic system used for grid generation.

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